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| Species Tag: | 42007 | Species Name: | CH3C-13-N |
| Version: | 1 | | Acetonitrile, |
| Date: | April 1996 | | ¹³ C on cyanide isotope |
| Contributor: | J. C. Pearson | | |
| Lines Listed: | 8951 | Q(300.0)= | 30370.2787 |
| Freq. (GHz) < | 1824 | Q(225.0)= | 19721.7674 |
| Max. J: | 99 | Q(150.0)= | 10734.5468 |
| LOGSTR0= | -10.0 | Q(75.00)= | 3797.4978 |
| LOGSTR1= | -10.0 | Q(37.50)= | 1347.9284 |
| Isotope Corr.: | -1.955 | Q(18.75)= | 493.1997 |
| Egy. (cm ⁻¹) > | 0.0 | Q(9.375)= | 192.3824 |
| μ_a = | 3.92197(13) | A= | 158093.3 |
| μ_b = | | B= | 9194.35 |
| μ_c = | | C= | B |

The experimental measurements are from: D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659., S. G. Kukolich, G. Lind, M. Barfield, L. Faehl, and J. L. Marshall, 1978, J. Am. Chem. Soc. **100**, 7155., S. G. Kukolich, 1982, J. Chem. Phys. **76**, 97., and J. C. Pearson and H. S. P. Müller, 1996, Astrophys J. Lett., submitted.

The details of the analysis are presented in the Pearson and Müller paper. The constants A, D_K , H_K cannot be determined from the microwave spectra and were determined by scaling the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spect. **157**, 198, and M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spect. **152**, 377 by the ground state average (r_z) structure differences from normal species. Other higher order constants (H_J , L_{JJK} , L_{JK} , L_{KKJ}) were fixed to scaled from the normal species (tag 41001).

The dipole moment was fixed to the main isotope reported by J. Gadhi, A. Lahrouni, J. Legrand, and J. Demaison, 1995, J. Chem. Phys. **92**, 1984.